# Macromolecules

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# Perspective

Research in Macromolecular Science: Challenges and Opportunities for the Next Decade

C. K. Ober,  $^{\dagger}$  S. Z. D. Cheng,  $^{\ddagger}$  P. T. Hammond,  $^{\$}$  M. Muthukumar,  $^{\parallel}$  E. Reichmanis,  $^{\perp}$  K. L. Wooley,  $^{\sharp}$  and T. P. Lodge\*,  $^{\nabla}$ 

Department of Materials Science and Engineering, Cornell University, Ithaca, New York 14853; Department of Polymer Science, University of Akron, Akron, Ohio 44325; Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139; Department of Polymer Science and Engineering, University of Massachusetts, Amherst, Massachusetts 01003; School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, Georgia 30332; Department of Chemistry and Department of Radiology, Washington University, St. Louis, Missouri 63130; and Department of Chemistry and Department of Chemical Engineering & Materials Science, University of Minnesota, Minneapolis, Minnesota 55455

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### Introduction

The broad field of macromolecular science has never been more vibrant. Driven by stunning fundamental advances in many fields, including (i) polymerization methods, (ii) theory, simulation, and modeling, (iii) understanding of new physical phenomena, (iv) advances in characterization techniques, and (v) harnessing of self-assembly and biological strategies for producing complex multifunctional structures, research activity in the field continues to expand and attract practitioners from many other disciplines. At the same time, society is confronted by global challenges that are coming into clear focus—the need for vast new and sustainable energy sources; the requirements for clean air, water, and food supplies; the need to supplement, reuse, and replace petroleum-based polymeric materials; demands for health care modalities that are enhanced both in efficacy and in affordability; technologies for improved security and defense. In all of these areas, new polymeric materials and new processes for polymers and polymer-containing composites will play crucial roles. Indeed, polymers arguably represent the most important class of materials today; their multiple and tunable attributes underpin expanding use across most advanced technology platforms.

In recognition of these huge challenges and associated opportunities, the National Science Foundation through the Polymers Program of the Division of Materials Research hosted a three-day workshop at NSF Headquarters in August 2007. The workshop was also cosponsored by the Air Force Office of Scientific Research, the Army Research Office, the Department of Energy (Basic Energy Sciences), the National Aeronautics and Space Administration, the National Institutes of Health (National Institute of Biomedical Imaging and Bioengineering), the National Institute of Standards and Technology, and the Office of Naval Research. Under the Chairmanship of Chris Ober, and with an organizing committee including Stephen Cheng, Paula Hammond, M. Muthukumar, Elsa Reichmanis, and Karen Wooley, over 50 participants (see Appendix) contributed to intense discussions, exchanges, and the preparation of a written report detailing a collective vision of challenges, goals, and strategies for the next decade. The full 120 pages of Interdisciplinary Globally-Leading Polymer Science & Engineering may be accessed via the Web (available at http:// www.nsf.gov/mps/dmr/reports.jsp), and we strongly encourage readers to take advantage of this collected wisdom. (Hard copies of the report may be obtained by request from Chris Ober at cko3@cornell.edu.) The purpose of this Perspective is not to supplant or duplicate the full report, but rather to highlight its

<sup>\*</sup> To whom correspondence should be addressed. E-mail: lodge@umn.edu.

<sup>†</sup> Cornell University.

<sup>&</sup>lt;sup>‡</sup> University of Akron.

<sup>§</sup> Massachusetts Institute of Technology.

<sup>&</sup>quot;University of Massachusetts.

Georgia Institute of Technology.

<sup>#</sup> Washington University.

<sup>&</sup>lt;sup>∇</sup> University of Minnesota.

existence and to re-emphasize some of the salient conclusions, quite possibly to a much broader audience. Our focus here is exclusively on research topics and on the exciting opportunities that lie before us. The report itself also details very useful suggestions for the polymer field in terms of education, outreach, broadening participation, and maintaining competitiveness; we do not address these issues here. We also wish to emphasize that the points made in this Perspective represent the views of the authors, as informed by the full report. It should not be construed as a blueprint for what should or should not be funded, nor should omission of any particular topic be taken to imply a considered judgment that it is not interesting or important.

# Societal Challenges and the Role of Polymer Science

The panel identified five broad areas where societal needs pose huge technological challenges and where polymer science must play a crucial role: energy, sustainability, health care, security and informatics, defense and protection. In fact, more than any other class of materials, polymers have the ability to serve in many different capacities, from major structural components (e.g., the upcoming Boeing 787 "Dreamliner" is 80% by volume carbon fiber reinforced thermoset) to high valueadded ingredients on the scale of grams (e.g., lithography, drug delivery). This versatility in applications stems directly from versatility in physical properties, which in turn reflects collective advances in molecular synthesis and design, in understanding the relationships between molecular architecture and material response, and in efficient processing strategies. In order to serve these diverse societal needs, the use of advanced polymer materials will have to expand into areas where more traditional materials predominate; success will therefore require continued, rapid progress in what polymer science can deliver.

In the field of energy, polymers will serve at least three broad functions: as components in new energy generating and storage systems, as lightweight structural materials that reduce fuel consumption, especially in transportation, and as more efficient platforms for separation technologies. In the first role, photovoltaics, fuel cell membranes, and battery separators are all areas of intense interest, especially when portability is important; yet, substantial materials challenges remain to be overcome. In the second, there remains significant opportunity to reduce mass in planes, trains, and automobiles. Third, industrial scale separation of liquids and gases is often extremely energy intensive, and next generation polymer membranes should offer substantial savings.

Disposable plastic packaging is ubiquitous in developed countries, fulfilling many important functions while also representing the archetypical example of waste and pollution. A greener polymer industry will not only provide biodegradable materials, but a broad suite of polymeric materials based on renewable feedstocks. Examples include both monomers prepared from biomass (e.g., lactic acid) and polymers and polymer composites derived directly from abundant biomaterials such as cellulose, starch, lignin, and chitin. Even petroleum-based polymers, the mainstay of current and near future macromolecular materials, can be made greener in terms of their synthesis and processing, for example by elimination of volatile organic solvents, by catalyst recycling and recovery, by more active catalysts, and by greener routes to purified monomers.

Polymers already feature in numerous biomedical applications, including drug delivery systems (e.g., coated stents, transdermal patches, polymeric micelles and nanoparticles), artificial replacements (e.g., hip, heart, prostheses), and tissue engineering. Nevertheless, the opportunities for more varied and more sophisticated applications are vast. In particular, one can envision moving beyond the current paradigm, in which the polymeric component tends to be designed to be passively tolerated by the organism for a sufficient time interval to serve its function, to one where the polymers have multiple functionalities, distributed over a hierarchy of length and time scales, to enable active interactions with cells and cellular control systems.

Although the current "information age" has brought many conveniences, it has also opened the door to new threats to the security of individuals and societies. In principle, polymers enable the high volume production of low cost and portable devices that can be used, e.g., as sensors or as identification systems. Functional enablement will require advances in synthesis, characterization, and basic understanding of optoelectronic polymers that can be readily incorporated into hybrid systems. Information gathering, storing, verification, and display are examples of functions that such systems must accomplish. A related challenge is to secure safe and sustained distribution of clean water. Polymers will play strategic roles in detection of toxins, in purification, and in storage. Defense applications for advanced polymer materials also abound, ranging from the demands placed by complex, multimillion dollar vehicles and aircraft to the protective gear issued to individual soldiers.

# **Interdisciplinary Polymer Science**

Polymer science has achieved a certain level of maturity over the past 60 years. For example, we have a deep understanding about the behavior of a solution or melt of monodisperse, flexible, uncharged, linear homopolymer chains. Yet, this knowledge does not mean the end of intellectual challenges in polymer science, but quite the opposite; increasingly, we are interested in more complex systems, including mixtures of polymers with polymers or polymers with particles, block polymers, branched polymers, charged systems, and rodlike molecules, to name only a few. The collective past achievements of the community will enable future progress across a much broader span of problems and solutions involving macromolecules. This breadth will inevitably heighten the importance of the interdisciplinary approach. Within polymer science itself, therefore, we envision a need for greater collaboration among those pursuing traditionally distinct areas: design and synthesis; characterization and properties; processing; theory and modeling. Perhaps even more importantly, collaboration of polymer science with other areas of chemistry, chemical engineering, materials science, physics, biology, biomedicine, cyber science, and environmental science holds tremendous promise.

### Synthesis of New Molecules and New Materials

The past decade has seen remarkable advances in our ability to prepare polymers with improved control over such molecular attributes as branching and architecture, chain length distribution, stereoregularity, copolymer composition, block polymer sequence and chain length, and precisely located functional groups. In many cases the newer protocols are relatively straightforward to implement and scale up, even while yielding more sophisticated materials. However, this burst of progress is likely only the beginning, and many more exciting developments should emerge. To address the grand challenge of "tailor-made materials", the panel identified eight general goals for the next 10 years. These may be briefly summarized as follows:

• Increased Synthetic Precision, which includes both the development of higher yield, "atom-efficient" syntheses and incorporation of orthogonal chemistries whereby the specific

- Precise Control of Heterogeneity and Multiple Functionality, whereby polymers containing multiple monomers and specific functional or responsive groups can be reliably prepared. Both this goal and the previous one offer exciting challenges for catalyst design.
- Simple and Robust Protocols for Complex Architectures. Star, comb, cyclic, hyperbranched, dendritic, and other nonlinear architectures have been the focus of much research, but in many cases the syntheses are elaborate and/or involve multiple steps. The application of such appealing macromolecules will be greatly facilitated by the development of simpler synthetic routes that are more amenable to scale up.
- Self-Replicating/Templating with Error Correction. This represents one of several themes in which polymer synthesis strives to learn from, and imitate, natural systems, whereby highly complex macromolecules such as proteins are built up step-by-step, yet flawlessly.
- Advanced Molecular Recognition and Noncovalent Assembly. Supramolecular interactions, i.e. those between covalent molecules, have been utilized to produce a variety of adaptive, self-healing, and stimuli-responsive materials, but the scope of opportunities is tremendous. Understandably, hydrogen bonding has been a popular supramolecular design element, but molecular recognition, ionic and electrostatic interactions, metal—ligand coordination, and hydrophobic/hydrophilic domains are all potentially rich routes to noncovalent polymer structures and materials.
- Hybrid Materials. Systems comprising mixtures of polymers and other materials, such as organic and inorganic additives, metals and metal clusters, nanoparticles, nanofibers, and mineral sheets, are increasingly touted for their superior properties. Yet, generally, the polymeric components have not been designed explicitly to control interactions with the other ingredients. There is also a need for a more "wholistic" design of nanocomposites, whereby both polymeric and nonpolymeric components are viewed as reagents in a single synthesis.
- Improved Conjugated Polymers. Conjugated polymers, or more broadly polymers that are conducting, semiconducting, light emitting, or absorbing, are essential ingredients in a host of advanced applications. Such materials are often tricky to prepare, especially by the controlled polymerization routes necessary to achieve, e.g., block polymers. Furthermore, conjugation is usually accompanied by conformational rigidity, which tends to inhibit solubility, which in turn impedes both molecular characterization and materials processing.
- Reduced Environmental Impact. This goal applies across the board, from the use of renewable feedstocks, the efficiency of the synthesis in terms of energy input and overall yield, the replacement or minimization of volatile organic compounds, to the degradability or recyclability of the final product.

# **Complex Polymer Systems**

The manipulation of secondary interactions, in addition to other thermodynamic and kinetic driving forces, can enable the generation of more complex polymeric materials. Such systems include block and heterocopolymers and their assembly in the bulk and in solution, but also an increasingly larger set of organic—inorganic or organometallic systems, supramolecular networks, and hybrid functional materials, many with nano- to micron-scale hierarchy. Often the controlled combination of macromolecular systems leads to dynamic or responsive materials. A greater understanding of how to induce and control these

interactions will ultimately lead to an expanded range of applications for polymers in medicine and several technologically demanding fields. In particular, energy transformation and storage applications represent a grand challenge for complex systems, due to the opportunity to address issues such as electronic carrier transport and catalytic activity in the form of low-cost, lightweight, and flexible films and coatings. The panel highlighted several key advances needed or anticipated in such complex polymer systems:

- Biomacromolecules as Models for, or Components of, Complex Polymers. While self-assembly of synthetic polymers tends to rely on dispersion forces, biology uses many other motifs for guiding structure, including helix- and sheet-forming peptide sequences. By orchestrating an ensemble of weak interactions, living systems produce high-strength materials (e.g., bone, skin, shells, and silk), biorecognition and catalytic specificity, and efficient energy harvesting. As polymer design and synthesis begins to replicate this sophistication, the need to better control the assembly of these systems to achieve the efficacy of nature-based design becomes significant. This is particularly pertinent in the extrapolation of two-dimensional structures to three-dimensional materials that can provide mechanical, biochemical, and structural cues to living systems for biomaterials and medicine.
- Reactive Systems driven by a single chemical reaction, or a series of events triggered by a chemical change, can yield new polymers that exhibit a broad range of stimuli-responsive behavior. Examples include photoresponsive macromolecular conformational changes and light- and temperature-induced changes in swelling, wetting, bulk or thin film morphology, and mechanical properties.
- Hierarchical Structures Using Charges provide new opportunities along with new challenges that must be met in order to access high levels of order. Controlled multilayer assembly methods combine different polymer backbones in nanoscale blends that would not ordinarily generate stable mixtures to form a broad range of inorganic/organic hybrid materials with controlled composition. The ability to manipulate the morphologies of these systems using interdiffusion of charged species during assembly, and concomitant manipulation of additional interactions such as hydrogen bonding, may lead to more complex morphological structure within the film. Difficulties persist in that positive and negative species can undergo undesired aggregation or complexation. The use of sophisticated chemistries could lead to charged groups that can be concealed or revealed only at desired times. Methods of manipulating charge include electrochemical reduction or oxidation, generation of charge in sequential or gradient fashion, tuning charge density along polymer backbones, and pH responsive or cleavable groups. Polymeric species play a special role in generating such complexes due to their multivalent nature and broad range of available architectures.
- Controlled Reversibility of Assembly. Adaptive structures can be realized through the manipulation of complementary interactions between polymer chains or polymers with other nanoscale elements, from nanoparticles to organometallic complexes or ligands. Such materials may undergo significant changes in mechanical properties or rheological behavior and could lead to responsive networks that undergo assembly and disassembly on command or in response to an environmental stimulus. Truly reversible assembled materials could enable responsive or adaptive membranes, drug delivery vehicles, biomedical materials, and active protection applications. General

challenges include hysteresis, cyclability, kinetic trapping of states, controlled sensitivity to the stimuli of interest, and the ability to drive assembly even under fairly dilute macromolecular concentrations.

- Complex Systems as a Route to Fabrication of Nanoscale Objects. Certain nonsymmetric or patterned nanoparticles are of great scientific and technological value but can be very difficult to prepare using traditional fabrication techniques. Complex polymer systems, from di- and triblock copolymers to hierarchical self-assembled structures, can be used to generate spherical, rodlike, tubular, and layered structures. A broader range of new structures can be generated by taking advantage of chemical composition differences within block polymer systems or by generation of highly specific and spatially localized regions during colloidal assembly. The ability to generate more diverse nanoparticle systems could provide components of devices that yield significant advances in targeted drug delivery, photonics, or catalytic and energy applications.
- Directing Structure via Controlled Kinetic Pathways. The more complex polymer systems that have been developed include supramolecular structures resulting from ionic, hydrogen bonding, hydrophobic, van der Waals, and other noncovalent interactions; assembly of these systems often yields structures that are actually kinetically trapped states. The ability to access kinetic states predictably could lead to an even broader range of useful structures.

## **Characterization and Properties**

Advances in synthetic techniques and in polymer functionality both require and inspire advances in our ability to characterize molecular and material structure in detail. The material properties in the final (usually solid) state, and the dynamic response in the states (usually liquid) used in both molecular characterization and processing, also must be understood to enable rational advances in polymer design and optimization of performance. The panel identified seven broad challenges that offer multiple opportunities for future research and development. These include the following:

- Heterogeneity in Multiple Variables. Detailed polymer characterization is hindered by the fact that the molecular species are generally heterogeneous in several characteristics, such as chain length, stereo- and regiochemistry, architectural perfection, and copolymer composition. The most successful strategy so far has been to draw on multiple techniques, but this is both time-consuming and limited. For example, while size exclusion chromatography may yield information on chain length distribution and NMR spectroscopy provide details on average composition and regiochemistry, how composition varies from chain to chain can only be assumed. Continued development of techniques with higher resolution (such as MALDI mass spectrometry and temperature gradient interaction chromatography) will pay dividends, as will application of tandem strategies, whereby high-resolution separation in terms of one variable is interfaced directly to high-resolution analysis of another.
- Properties of Individual Chains. The ultimate in resolution is measurement on single molecules. This has already been achieved in certain cases, such as the force versus extension response of single DNA molecules and the visualization of molecular deformation in extensional flow or while undergoing electrophoresis. More generally, it would be profoundly exciting to measure other properties of single chains, including chemical sequence and structure or the response to various forces and interactions, and to be able to measure these under a variety of

environments (e.g., isolated molecules, within a bulk phase, at a surface or interface).

- Morphology. Polymers routinely display a rich variety of morphological features, including amorphous solid; crystalline and semicrystalline domains; networks and gels; liquid crystalline order and other mesophases; block polymer nanostructures; discrete and continuous phase-separated domains. To further complicate matters, two or more of these motifs often coexist and in a spatially heterogeneous way. Similarly, active research in polymer composites and hybrid materials provides new characterization challenges in terms of polymer structure under confinement or near hard interfaces with fibers, particles, platelets, and nanotubes.
- Multiple Length and Time Scales. Inherently, polymer molecules and polymer materials exhibit important structural features from the subnanometer range up to many microns. The powerful techniques currently available, for instance scattering and microscopy, tend to be limited in the available range or at least to require more than one instrument access the desired resolution. This limitation is even more prevalent in the time domain, where molecular motion occurs from at least the picosecond range (e.g., side group and solvent motion) up to arbitrarily long times (e.g., aging of a glass). Consequently, there is a general need for characterization tools with expanded dynamic range or for the simultaneous application of complementary techniques on a given sample.
- Real-Time, High-Throughput Characterization. In most cases molecular or materials characterization comprises a separate step after synthesis and/or processing. There are great opportunities for the development of techniques that can be applied in real time, in situ, to provide greater control over the synthesis or process, and for techniques that are amenable to high-throughput analysis given the emergence of synthetic polymer "libraries".
- Defects and Impurities. As polymers increasingly find application in nanotechnology and other demanding arenas, a general problem arises, essentially the proverbial needle in the haystack. Unintended variations in structural regularity ("defects"), dilute but nevertheless fatal levels of impurities, or even low level incorporation of intended heterogeneities present a characterization challenge. The tools at hand tend to present information on the predominant structural motif and are not sufficiently sensitive to minority components.
- Underutilization and Misapplication of Sophisticated Tools. There is a host of powerful characterization tools in regular use and readily accessible (at least in principle). Yet, there are obstacles to the full or appropriate utilization of such techniques. On the one hand, large-scale user facilities, such as those for small-angle neutron scattering and synchrotron X-ray scattering, may have open user programs and dedicated staff, but there can still be significant activation barriers for nonexperts to become proficient users. On the other hand, significant advances in the commercial availability of sophisticated instruments (e.g., rheometers, light scattering spectrometers) can have the unintended consequence of encouraging misuse, as the underlying subtleties and assumptions of the technique are forgotten in the apparent simplicity with which large amounts of data can be generated. The solution to both of these issues will rely on improved education more than on research per se, but of course, training of students is the cornerstone of academic polymer science.

# Theory and Simulations

Major advances in analytical theory, coupled with ever increasing computational power for simulations, have positioned

polymer theorists to play a major role over the next decade in guiding the synthesis, processing, and molecular design of polymeric materials. The panel delineated three "grand challenges": (i) to formulate the design rules for tailor-made materials, including hierarchical composites and biological hybrids; (ii) to understand the fundamentals of electronic, ionic, photonic, and energy transport in polymer systems from solar cells to living cells and from batteries to sensors and membranes; (iii) to formulate criteria for efficient and robust processing strategies, especially for complex structures. Within these broad issues, several more focused goals were highlighted:

- Electrically Charged Polymeric Systems. This class of macromolecules underpins an expanding set of new synthetic materials as well as encompassing most functional biological materials. Fundamental intellectual challenges abound in this arena, of which two, in particular, stand out. The first is the fact that the dielectric properties of the medium are spatially heterogeneous, which inherently compromises the mean-field approach that is so successful in other areas of polymer science. The second is that the operative length scales for electrostatic interactions are sufficiently large that they match and, therefore, couple to molecular conformations. In addition to these complications, it will be necessary to incorporate the multiplicity of interactions that nature routinely exploits into the theoretical picture, before the full sophistication of nature's smart and responsive materials can be designed into synthetic systems.
- Nonequilibrium Properties and Processes. It is often the case that polymeric materials do not achieve an equilibrium state; similarly, the processing of polymers usually involves strong flow, temperature gradients, and other fields that take the system far from equilibrium. This poses a huge challenge in terms of predicting the ultimate structure, at the nanoscopic, mesoscopic, and even macroscopic levels. It is impractical to develop a theory for the full free energy landscape, and there are generally many metastable states separated by substantial barriers. Thus, developing physical insight into the dominant pathways and factors will be key; such factors will likely be rather system specific. As the spatial and temporal scales are so broad in scope, multiscale modeling and appropriate coarse graining will be essential. Then, predicting or understanding structure is only the beginning; the relationship of structure to the mechanical and transport properties of interest remains the ultimate goal.
- Self-Assembly of Hybrid and Hierarchical Structures as Functional Objects. A significant fraction of contemporary polymer science exploits self-assembly as a guiding principle in producing nanostructured materials. This area is rich in theoretical challenges, beginning with the basic design rules for fabrication of supramolecular and hybrid structures. This entails, inter alia, the selection of interactions that will guide the assembly, the architecture of the polymeric components, and the choice of processing strategy to achieve the desired structure. There is also a great need for predictive theory; theory must be able to guide the synthesis in order to achieve the desired morphologies and phase behaviors, not just explain post facto the phenomenological results.
- Photonic, Ionic, and Electronic Materials. Key technological goals such as more efficient photovoltaics, more effective fuel cell membranes, and more reliable water purification will all be facilitated by deeper understanding of charged moieties, ions, excitons, and molecular and gas transport in polymer materials. For example, better understanding of hole and electron mobilities and band structure will guide synthetic efforts and lead to improved polymer semiconductors, while facilitating exciton

transport will improve organic solar cells; both problems require a quantum mechanical treatment. Even in the classical domain, challenges remain in terms of identifying the ideal membrane structures for proton conduction.

- Synthesis. As the power of modern synthetic tools grows, there is an increasing need for theoretical input and collaboration, in large part because the scope of accessible polymer structures is now too vast for systematic mapping. For example, of all the possible nonlinear architectures that can be prepared, which one will be best for a particular application? If a small fraction of functional monomers are to be incorporated within a polymer chain, what fraction is the right fraction, and how should they be distributed? Given that even the most "controlled" polymerization schemes will lead to some heterogeneity of molecular variables, we need to understand the tolerance of the desired properties relative to the achievable synthetic precision. And, while the basic kinetic schemes for most polymerizations are well established under ideal conditions, such conditions rarely prevail in practice. A detailed understanding of polymerization kinetics is lacking for commercially important situations such as reaction during flow or in the presence of phase separation, crystallization, or cross-linking.
- Crystallization and the Glass Transition. These classic problems of polymer physics have seen substantial progress in theoretical understanding, yet significant challenges remain in both cases. Furthermore, advances in simulation and computation have been matched by advances in experimental technique, so that problems of immense practical importance such as flowinduced crystallization can now be attacked in detail. Another example of great interest is to understand more fully the relationships among (i) the chemical specificity of the macromolecule; (ii) segmental dynamics, or  $\alpha$ -relaxation, that herald the glass transition; (iii) chain dynamics, which determine viscoelastic response and mechanical properties; and (iv) thermal history, which establishes the particular nonequilibrium state.

# Macromolecular Processing and Assembly

Polymers are almost always processed in a liquid state, often far from equilibrium, and solidified by some combination of vitrification, crystallization, and cross-linking; the resulting metastable material exhibits history-dependent structure and properties. By skillful processing, a given polymer or family of polymers can be converted into a wide range of distinct materials, including fibers, films, coatings, and molded parts. Many significant advances in the past decade have featured some aspect of structural control on the nanoscale, a trend that is sure to expand. Nanofabrication of polymer materials increasingly exploits a combination of top-down strategies, such as lithography, with bottom-up methods such as self-assembly. Within this extremely fertile area, two grand challenges emerged. The first is to achieve precision fabrication of both two- and threedimensional materials, with nanometric control; this includes both regular and aperiodic structures, and both large volume and very small scale processes. The second grand challenge is to develop ambient temperature, environmentally benign processes across a range of material platforms. While this goal has a clear sustainability benefit, it is also the case that many advanced polymer materials for, e.g., electronic or biological applications, cannot withstand the high-temperature processing typical of commodity thermoplastics.

The panel also identified several more targeted needs, including the following:

• Innovative Processing for Nanostructured Materials. The precision of lithography at the tens of nanometer scale is the cornerstone of the microelectronics industry, but the need for smaller features exceeds current processing (and materials) capability. The use of block polymer self-assembly is just emerging as one innovative processing route, including substrate-pattern or template-directed self-assembly, but the field is wide open for new approaches and for a whole host of applications beyond microelectronics.

- Precision Fabrication in Three Dimensions. It is highly desirable to extend the precision of two-dimensional lithographic patterning to true three-dimensional structures, but repetitive scanning/developing/fixing steps can be prohibitive. Self-assembly alone can produce three-dimensional structures, but only with a limited set of symmetries. Thus, innovative approaches that combine top-down with bottom-up processes hold much promise.
- Processing of Complex Organic/Inorganic Systems. The property advantages offered by such hybrid materials has stimulated huge activity in this area, but processing (for example, even to produce something as conceptually simple as a homogeneous dispersion of nanoparticles or nanowires) has proven remarkably difficult. Achieving higher order control, such as prescribed orientation, is, therefore, an even greater challenge.
- Low-Temperature, Environmentally Benign Processing. Identified above as a grand challenge, there are many specific goals to be achieved, including low-temperature processes for sensitive materials; energy efficient processing; elimination of volatile organic compounds from conventional processing; improved recyclability, for example by judicious choice of additives and processing aids such as nucleators, pigments, and mold release agents.
- In-Situ, Real-Time Process Monitoring. This general goal was also touched on under Characterization and Properties. There are two aspects to this issue. The first is to develop improved means of characterizing heretofore poorly understood structure-formation processes. The second is to apply these in real time as process control aids. This is particularly important for the many future products that are likely to be "high value-added" polymer materials, which may be produced on smaller scales or in smaller batches.

# **Summary and Outlook**

In a recent study under the auspices of the Department of Energy, Office of Basic Energy Sciences (BES), entitled "Directing Matter and Energy: Five Challenges for Science and the Imagination", the significant challenges for the broad field of Basic Energy Sciences were formulated (the full report is available at http://www.sc.doe.gov/BES/reports/abstracts. html#GC). It is illuminating to compare these targets with those identified in the NSF Polymers Workshop and summarized here because although the BES report is necessarily much broader in scope, there are direct analogies in all cases. For example, the first BES grand challenge is:

- How do we control material processes at the level of electrons? This mirrors the basic goal of polymer science, where the manifestation of electronic structures on the monomer scale in polarizable media, and the ultimate electronic properties of assembled macromolecules, require thorough investigation and understanding. Similarly, the second grand challenge is:
- How do we design and perfect atom- and energy-efficient synthesis of revolutionary new forms of matter with tailored properties? This is directly analogous to the goal of increased synthetic efficiency and sustainability in polymer chemistry. The remaining three challenges could have been taken directly from the Polymers Workshop:

- How do remarkable properties of matter emerge from complex correlations of the atomic or electronic constituents, and how can we control these properties?
- How can we master energy and information on the nanoscale to create new technologies with capabilities rivaling those of living things?
- How do we characterize and control matter away—especially very far away—from equilibrium?

We contend that these parallels between the two reports are not coincidental, but reflect the breadth of polymer science, and how advances in understanding and controlling the properties of polymeric materials, via a synergistic collaborative approach among experimentalists and theorists, will ultimately contribute in substantial ways to all the technological challenges that confront modern society. The challenges are great, but the opportunities are vast; these are exciting times to work in macromolecular science.

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### **Appendix**

Invited participants in the workshop included the following:

Eric Amis (NIST)

Kristi Anseth (University of Colorado at Boulder)

Lynden Archer (Cornell University)

Shenda Baker (Harvey Mudd College)

Anna Balazs (University of Pittsburgh)

Zhenan Bao (Stanford University)

Frank Bates (University of Minnesota)

Brian Benicewicz (RPI)

Kurt Binder (University of Mainz)

William Brittain (Bausch & Lomb)

Ken Carter (University of Massachusetts Amherst)

Ralph Colby (Pennsylvania State University)

Monica Olvera de la Cruz (Northwestern University)

Joseph DeSimone (University of North Carolina at Chapel Hill)

Barry Farmer (AFRL)

Richard Friend (Cambridge University)

Mary Galvin (Air Products)

Jan Genzer (North Carolina State University)

Sharon Glotzer (University of Michigan)

Peter Green (University of Michigan)

Barney Grubbs (Dartmouth College)

Kathleen Havelka (Lubrizol Corp)

Craig Hawker (University of California at Santa Barbara)

Anne Hiltner (Case Western Reserve University)

Catherine Hunt (Rohm & Haas)

Kristi Kiick (University of Delaware)

Sanat Kumar (Columbia University)

Christopher Li (Drexel University)

Eric Lin (NIST)

Tim Lodge (University of Minnesota)

Lon Mathias (University of Southern Mississippi)

Kris Matyjaszewski (Carnegie Mellon University)

Jimmy Mays (University of Tennessee Knoxville)

LaRuth McAfee (Case Western Reserve University)

Scott Milner (Exxon Mobil)

George Newkome (University of Akron)

Christine Ortiz (MIT)

Michael Owen (Dow Corning, retired)

Stuart Rowan (Case Western Reserve University)

Rick Register (Princeton University)

Tom Russell (University of Massachusetts Amherst) Rachel Segalman (University of California Berkeley)

Sam Stupp (Northwestern University)

Doug Robello (Kodak)

Stuart Rowan (Case Western Reserve University)

Tim Swager (MIT) Ned Thomas (MIT) Dave Tirrell (Caltech)

Marek Urban (University of Southern Mississippi)

Zhen-Gang Wang (Caltech) Uli Wiesner (Cornell University)

Karen Winey (University of Pennsylvania) Shu Yang (University of Pennsylvania)

Federal Agency Participants
Paul Armistead (ONR)
Kathryn Beers (OSTP)
David Brant (NSF)
Kenneth Caster (ARO)
John Connell (NASA)
Lori Henderson (NIH/NIBIB)

Richard Kelley (DOE/BES) Freddy Khoury (NSF) Douglas Kiserow (ARO) Charles Lee (AFOSR) Andrew Lovinger (NSF) Michael Meador (NASA) Tyrone Mitchell (NSF) Arthur Snow (ONR) Chad Snyder (NIST) Robert Wellek (NSF)

Student Participants

Michelle Chavis (Cornell University) Nelson Felix (Cornell University)

Jodie Lutkenhaus (MIT)

Ryan Murphy (University of Massachusetts Amherst)

Renee Smith (MIT)

Brooke Van Horn (Washington University in St. Louis)

Bryan Van Horn (University of Akron)

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